Opacity Calculations at Los Alamos
or
Dark Doings on the Mesa

Norman H. Magee

Los Alamos National Laboratory
Los Alamos, NM 87545

Opacity calculations have been done at Los Alamos for more than 40 years. This has involved many people and a long series of opacity codes. During this period, there have been many inovations and changes as developers strove to take advantage of new physics models and improved computational facilities. One of the most important lessons learned during this evolution was the need for constant evaluation and comparison of results, especially as new models were included or as calculations were pushed into new physical regimes. Los Alamos has always tried to maintain two or more "independent" opacity codes to monitor all code changes, and while this is a necessary procedure, it is not sufficient to ensure the best opacity calculations. This can only be done by comparisons with experiment and with truly independent codes from other laboratories or groups. In the late 1980's, these both became realities with the start of the Opacity Workshops and the first quality transmission experiments at AWE. All current opacity codes have benefited from both of these developments, but the benefits have been limited because of the relativly small number of elements, temperatures and densities that have actually been compared or measured. While workshop cases are chosen to test critical regions, one or two test points can not predict error bars for the full temperature-density ranges covered by modern opacity tables. The next step forward for verification and validation will have to involve much more extensive comparisons among all of the major opacity codes, and include EOS as well as opacities.

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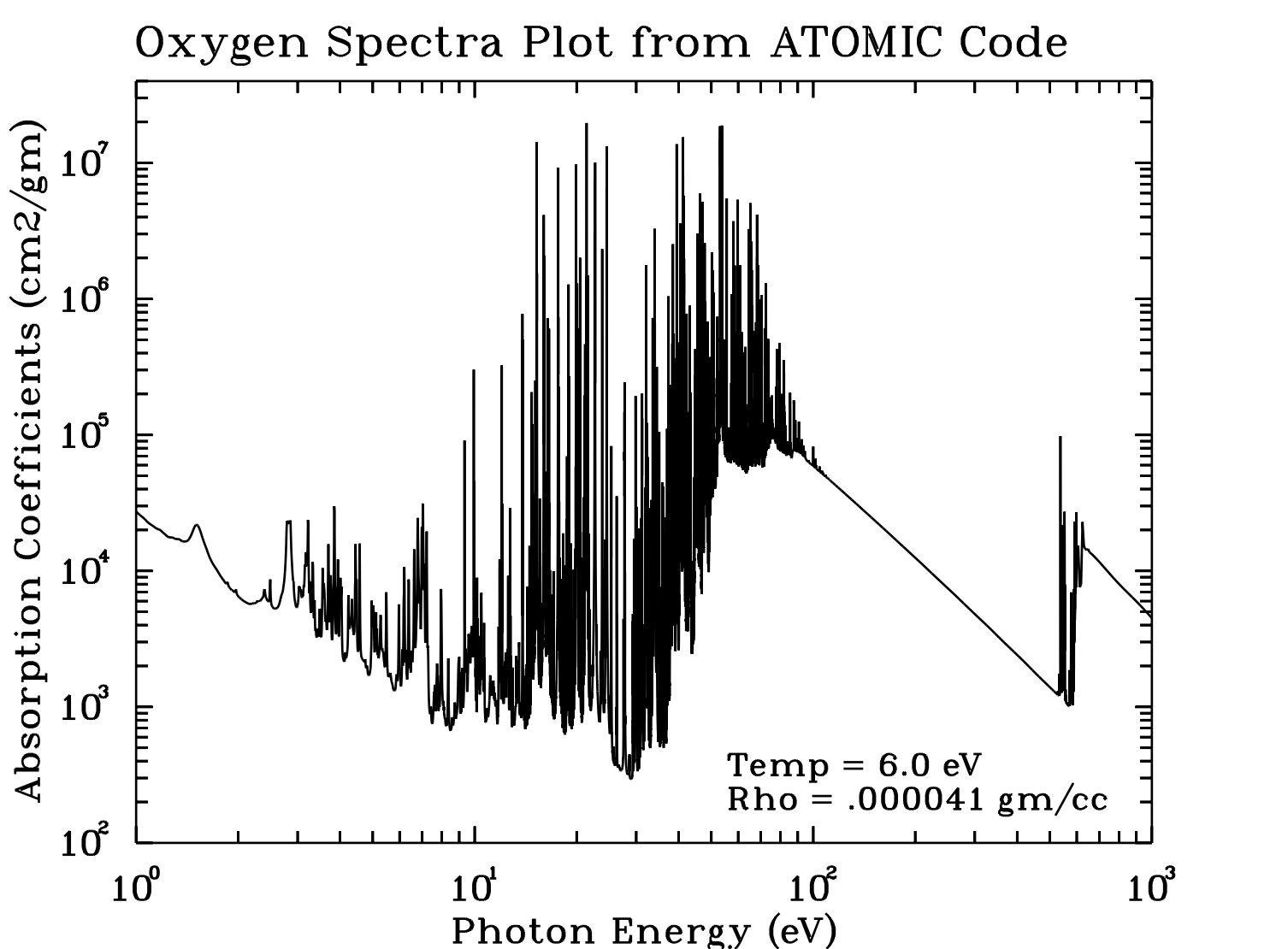
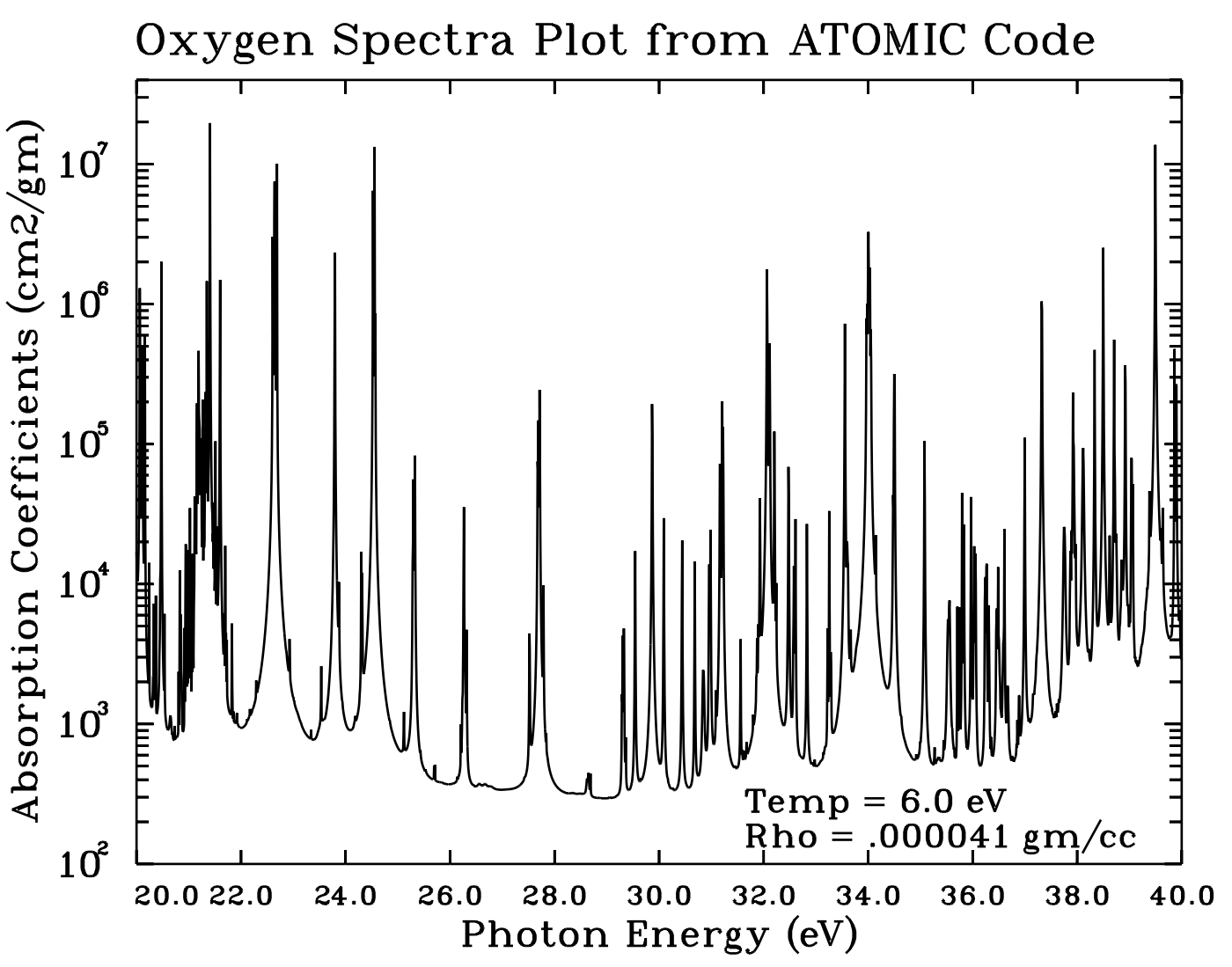
Atomic Physics, Opacity, Non-LTE and Spectra

Harris Mayer
Art Cox
Don Eilers
John Stewart
Dave Barfield
Doug Sampson
Bob Cowan
Joe Mann
Walter Huebner
Mary Argo
Al Merts

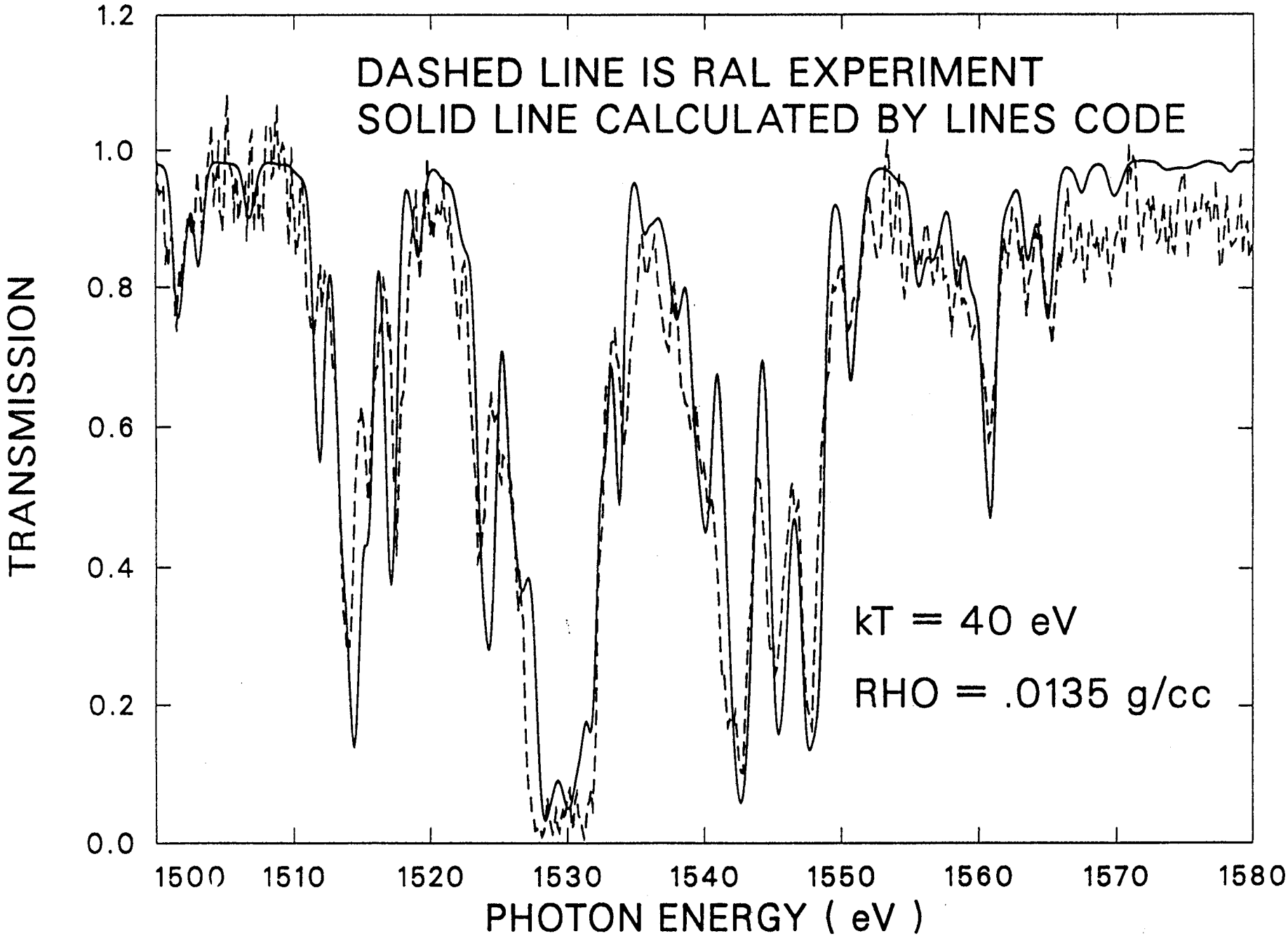
Norm Magee
John Keady
Carlos Iglesias
Bob Clark
Joe Abdallah
Chris Fontes
Honglin Zhang

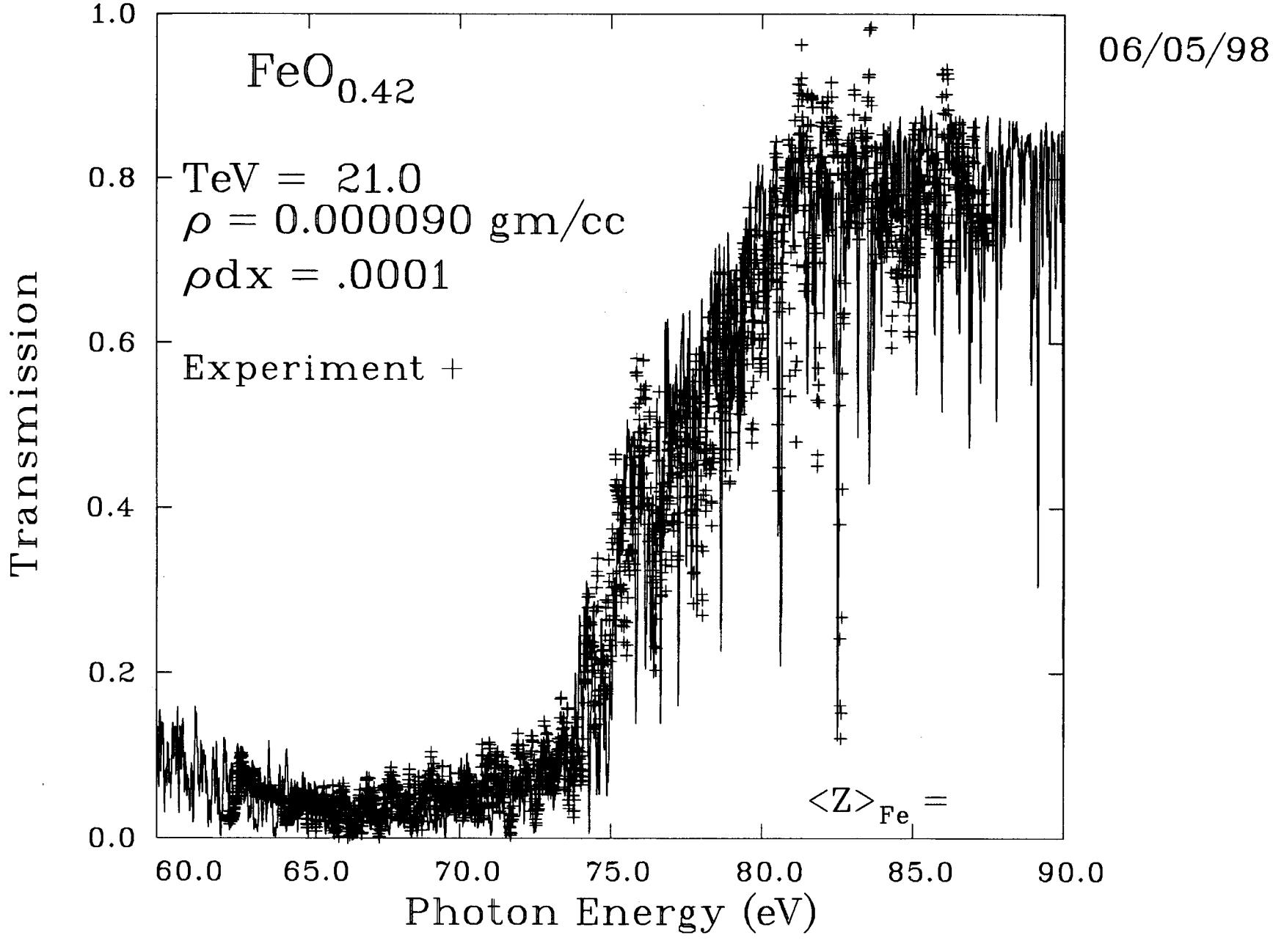
David Kilcrease
Stephane Mazevet
Lee Collins
Manolo Sherrill
Peter Hakel
James Colgan


Oxygen Spectra Plot from ATOMIC Code
Absorption Coefficients (cm2/gm)
10^7
10^6
10^5
10^4
10^3
10^2
10^0
10^1
10^2
10^3
Photon Energy (eV)
Temp = 6.0 eV
Rho = .000041 gm/cc


Oxygen Spectra Plot from ATOMIC Code
Absorption Coefficients (cm2/gm)
10^7
10^6
10^5
10^4
10^3
10^2
20.0 22.0 24.0 26.0 28.0 30.0 32.0 34.0 36.0 38.0 40.0
Photon Energy (eV)
Temp = 6.0 eV
Rho = .000041 gm/cc

ALUMINUM X-RAY TRANSMISSION




$FeO_{0.42}$
TeV = 21.0
ρ = 0.000090 gm/cc
ρdx = .0001
Experiment +
<Z>$_{Fe}$ =
06/05/98
Transmission
Photon Energy (eV)
1.0
0.8
0.6
0.4
0.2
0.0
60.0
65.0
70.0
75.0
80.0
85.0
90.0

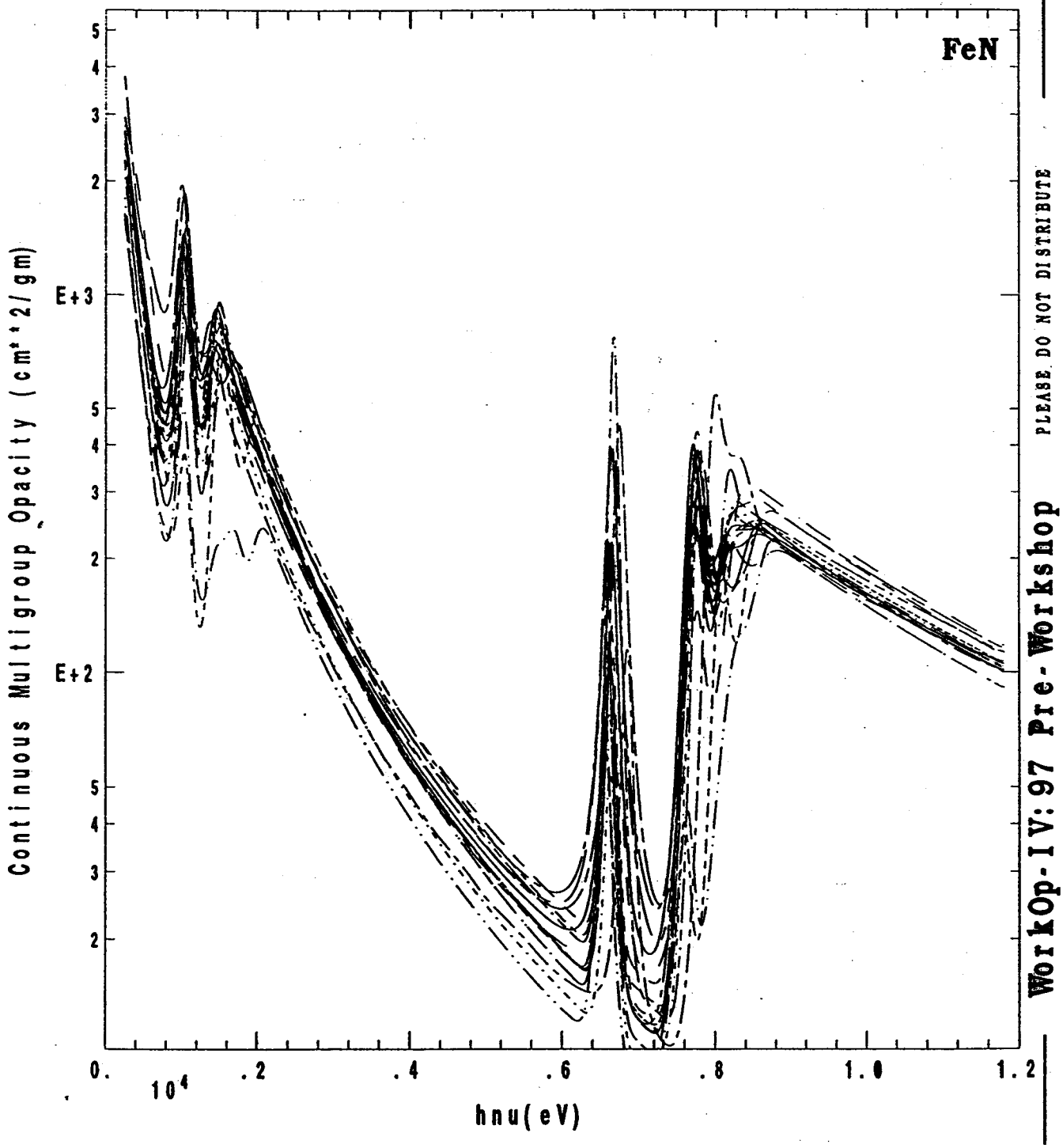
Continuous Multigroup Opacity (group width=kT/3) for FeN

Z=26 Rho = 8.0E+00 g/cc kT = 600. eV

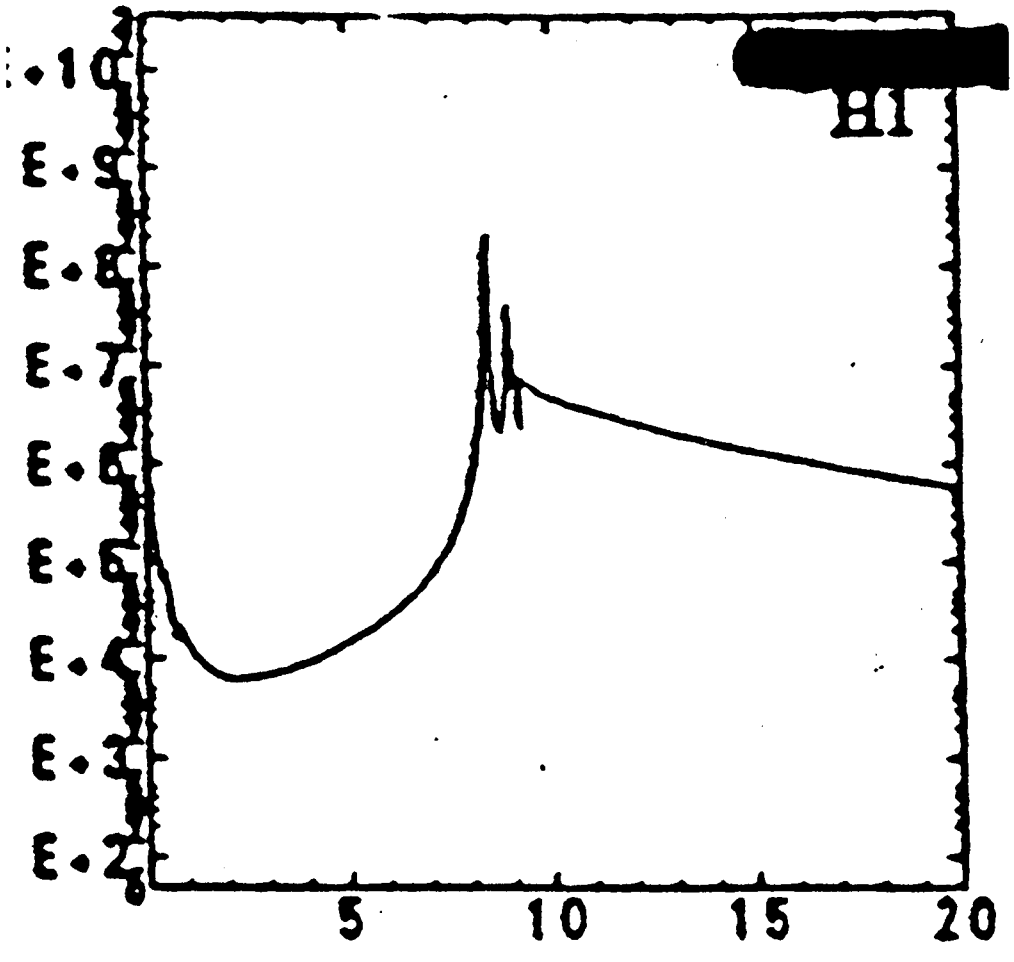
The Rosseland Mean of the Continuous Multigroup Opacity is identical, by construction, to the Rosseland Mean of the submitted total opacity.

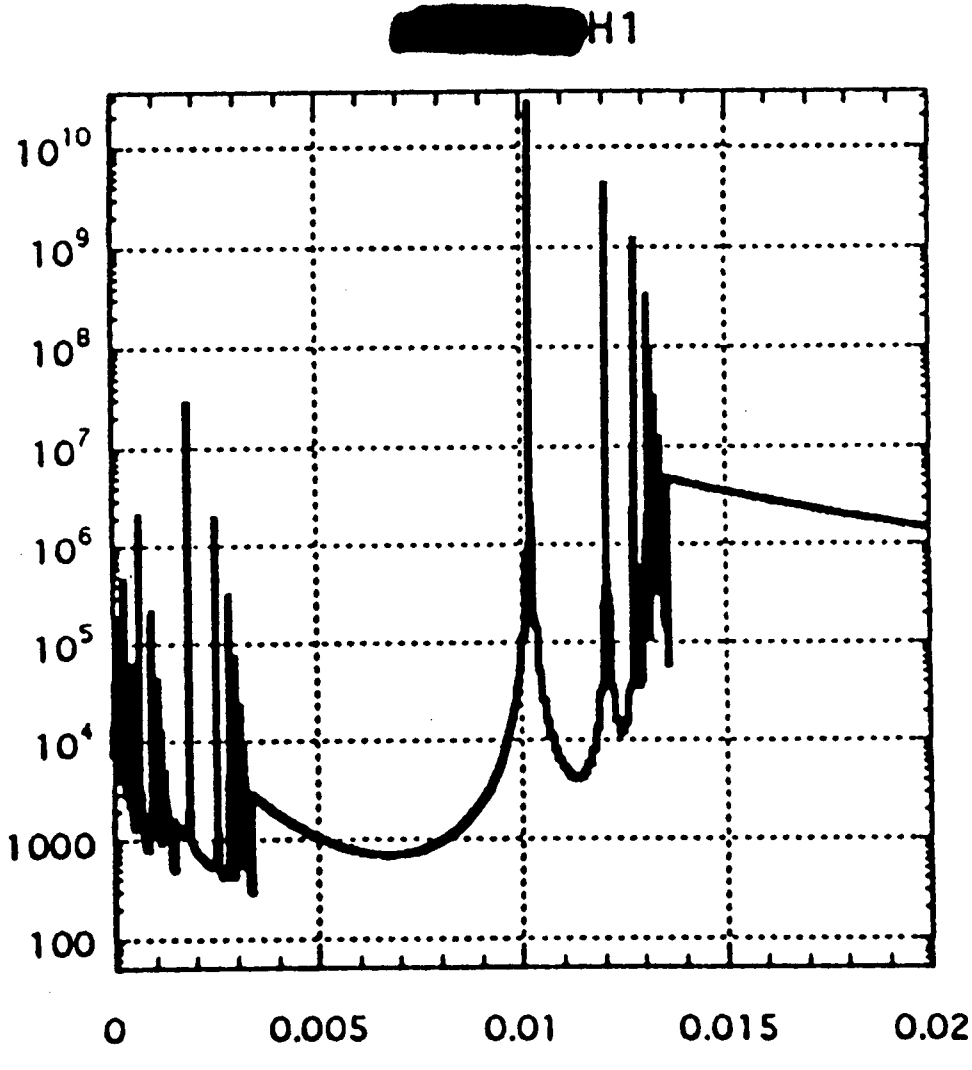
*** N.B. The Planck Mean and peak heights are NOT preserved. ***

Compare valleys and smooth portions. Disregard absolute peak heights.

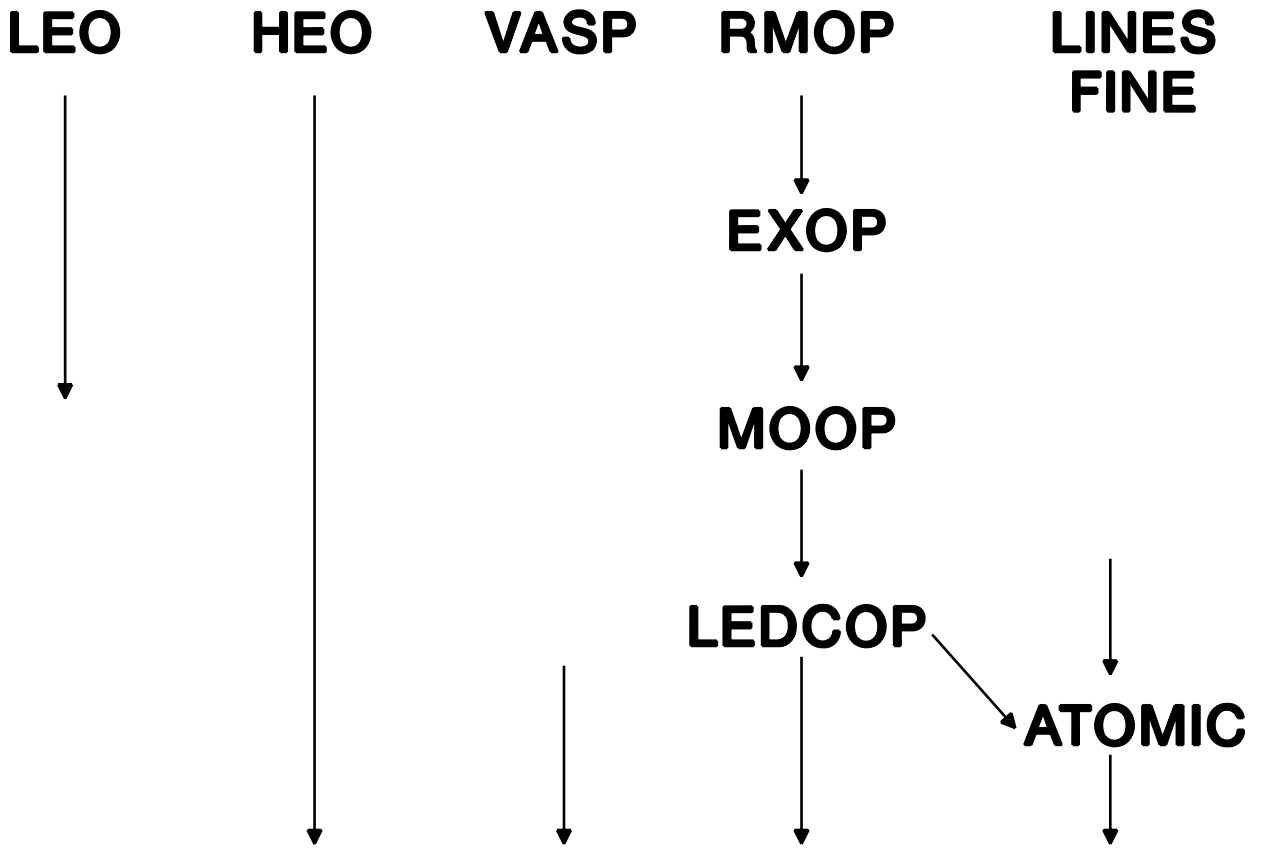


WorkOp-IV: 97 Pre-Workshop PLEASE DO NOT DISTRIBUTE


H1
5
10
15
20


H1
10^{10}
10^{9}
10^{8}
10^{7}
10^{6}
10^{5}
10^{4}
1000
100
0
0.005
0.01
0.015
0.02

Los Alamos Opacity Codes



The Making of *ATOMIC*

FINE

Spectral modeling code

Direct access to atomic physics data (*CATS, RATS, GIPPER, ACE*)

Bound-bound & bound-free cross sections

LTE & non-LTE

Low & high Z

+

LEDCOP

Free-free

Scattering

Stark broadening

Conductive opacity

Line shapes

+

new

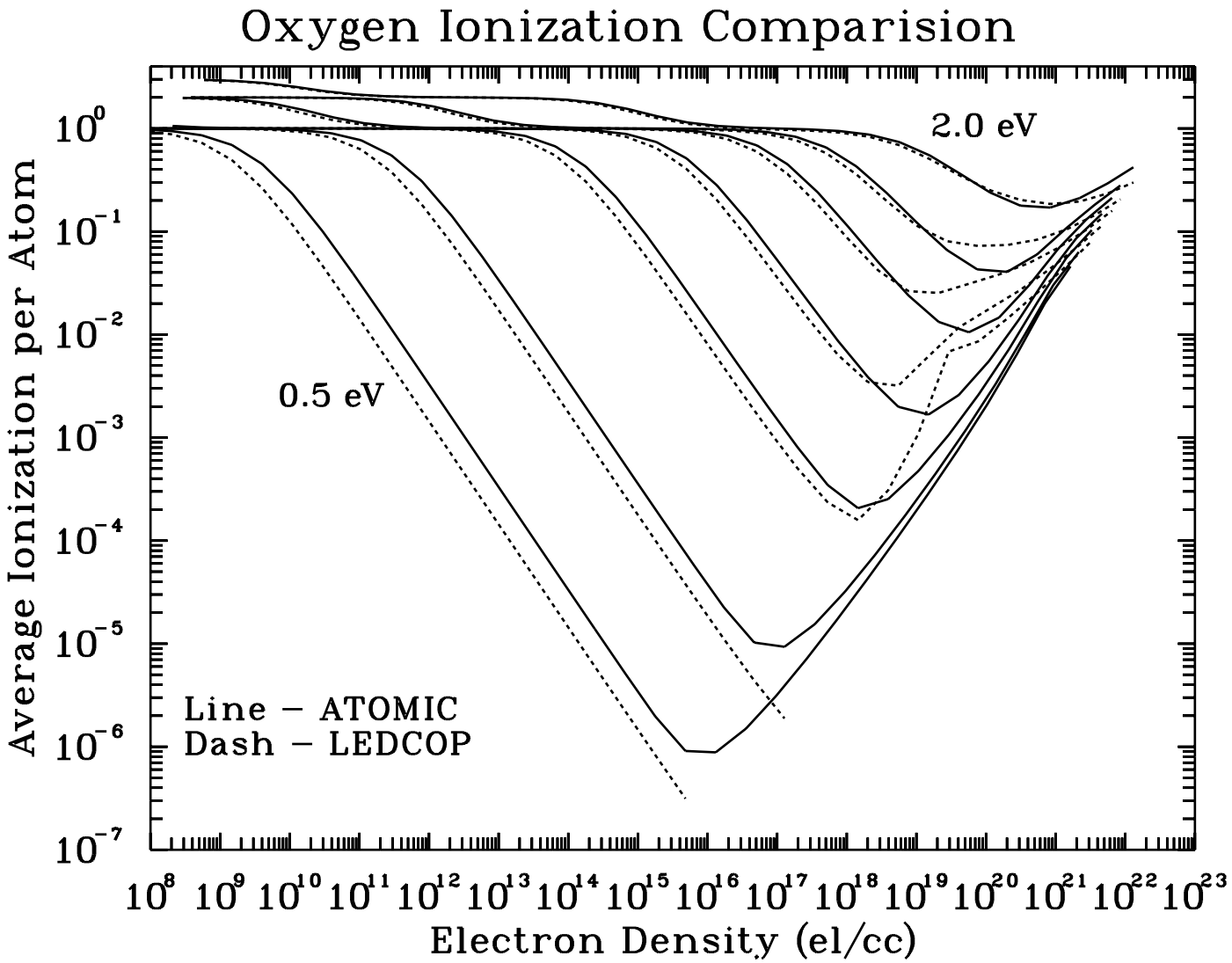
F90

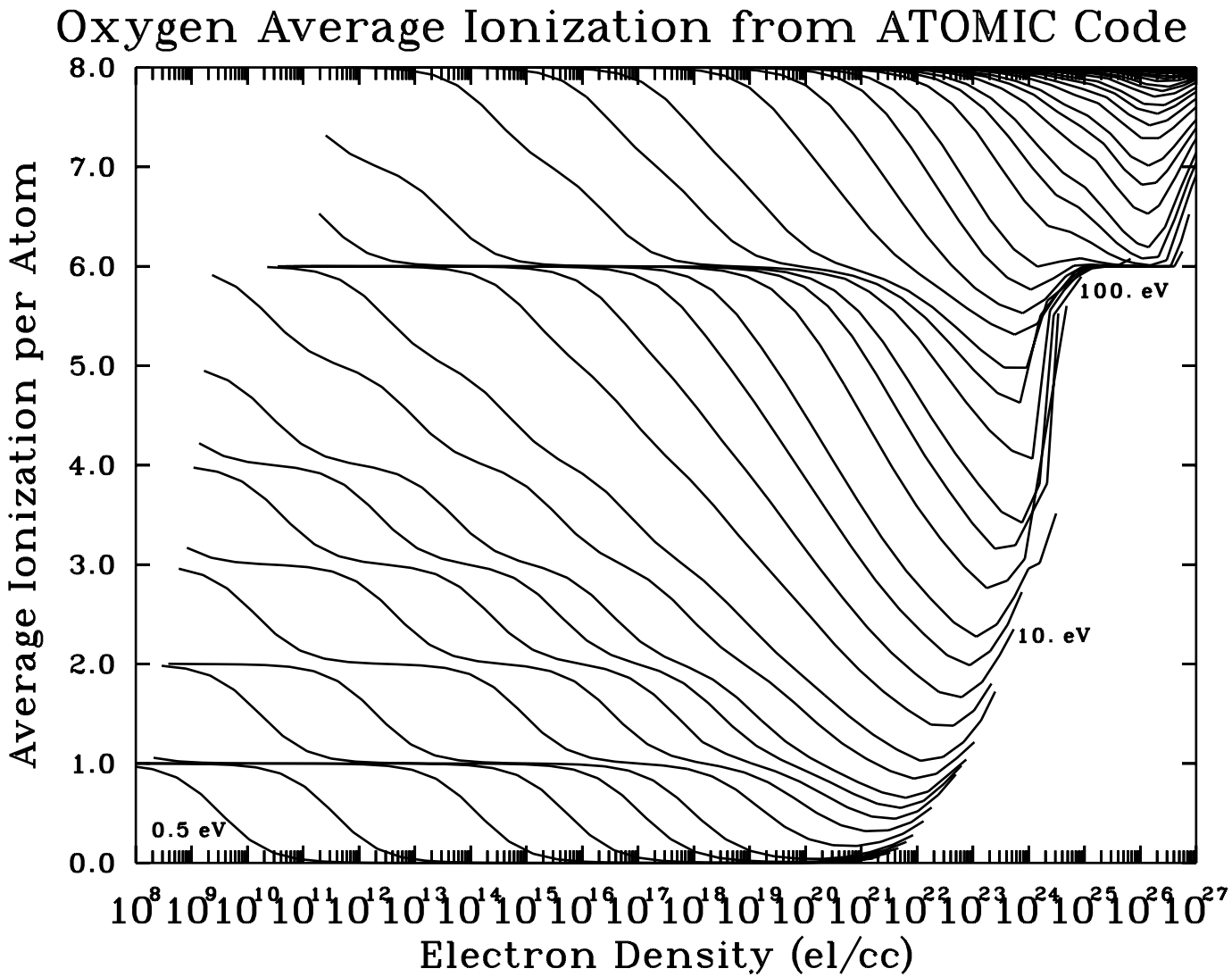
Parallelization

EOS

Line-edge merging

Histograms

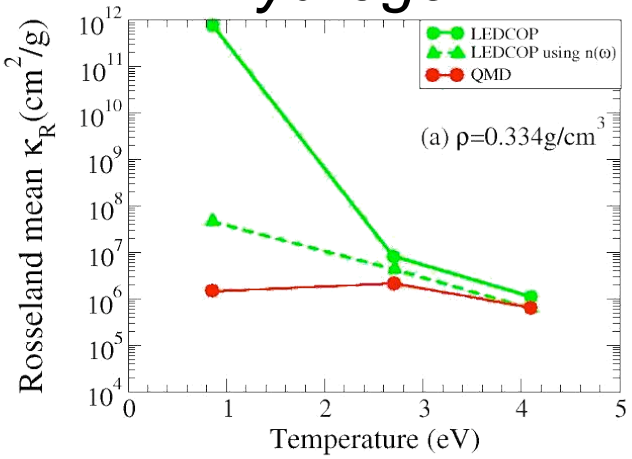

Oxygen Ionization Comparision
Average Ionization per Atom
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
2.0 eV
0.5 eV
Line – ATOMIC
Dash – LEDCOP
10^{8} 10^{9} 10^{10} 10^{11} 10^{12} 10^{13} 10^{14} 10^{15} 10^{16} 10^{17} 10^{18} 10^{19} 10^{20} 10^{21} 10^{22} 10^{23}
Electron Density (el/cc)

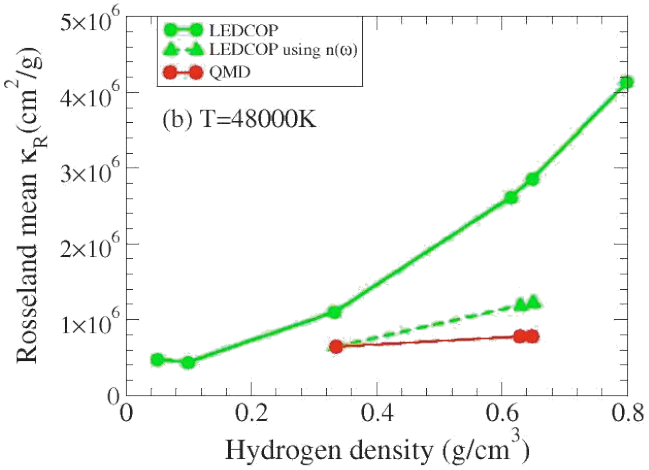

Oxygen Average Ionization from ATOMIC Code
Average Ionization per Atom
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
100. eV
10. eV
0.5 eV
10^8 10^9 10^10 10^11 10^12 10^13 10^14 10^15 10^16 10^17 10^18 10^19 10^20 10^21 10^22 10^23 10^24 10^25 10^26 10^27
Electron Density (el/cc)

QMD for Opacities

Comparison to *LEDCOP*

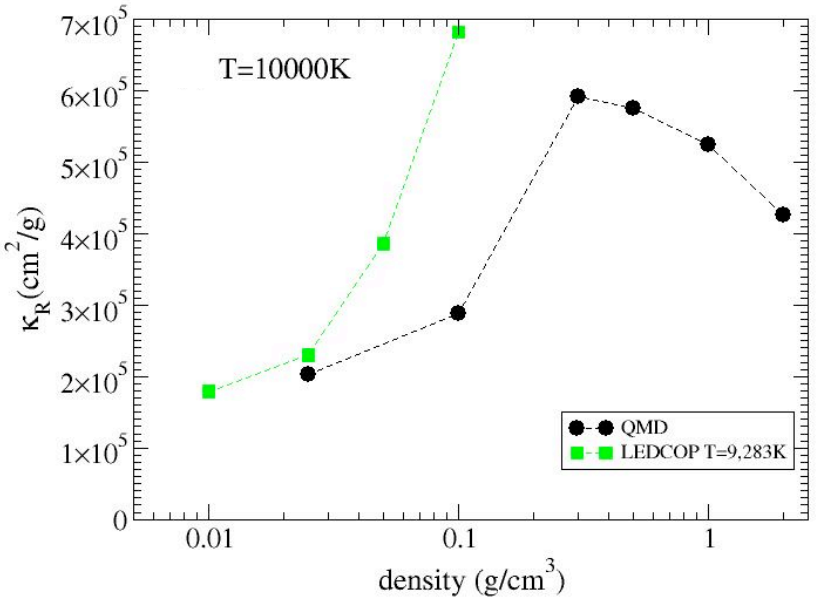
Hydrogen





S. Mazevet *et al*, Astron. Astrophys. **405**, L5 (2003)

Aluminum



S. Mazevet *et al*, Phys. Rev. E **71**, 016409 (2005)

Los Alamos NATIONAL LABORATORY

ATOMIC & OPTICAL THEORY T-4 LOS ALAMOS

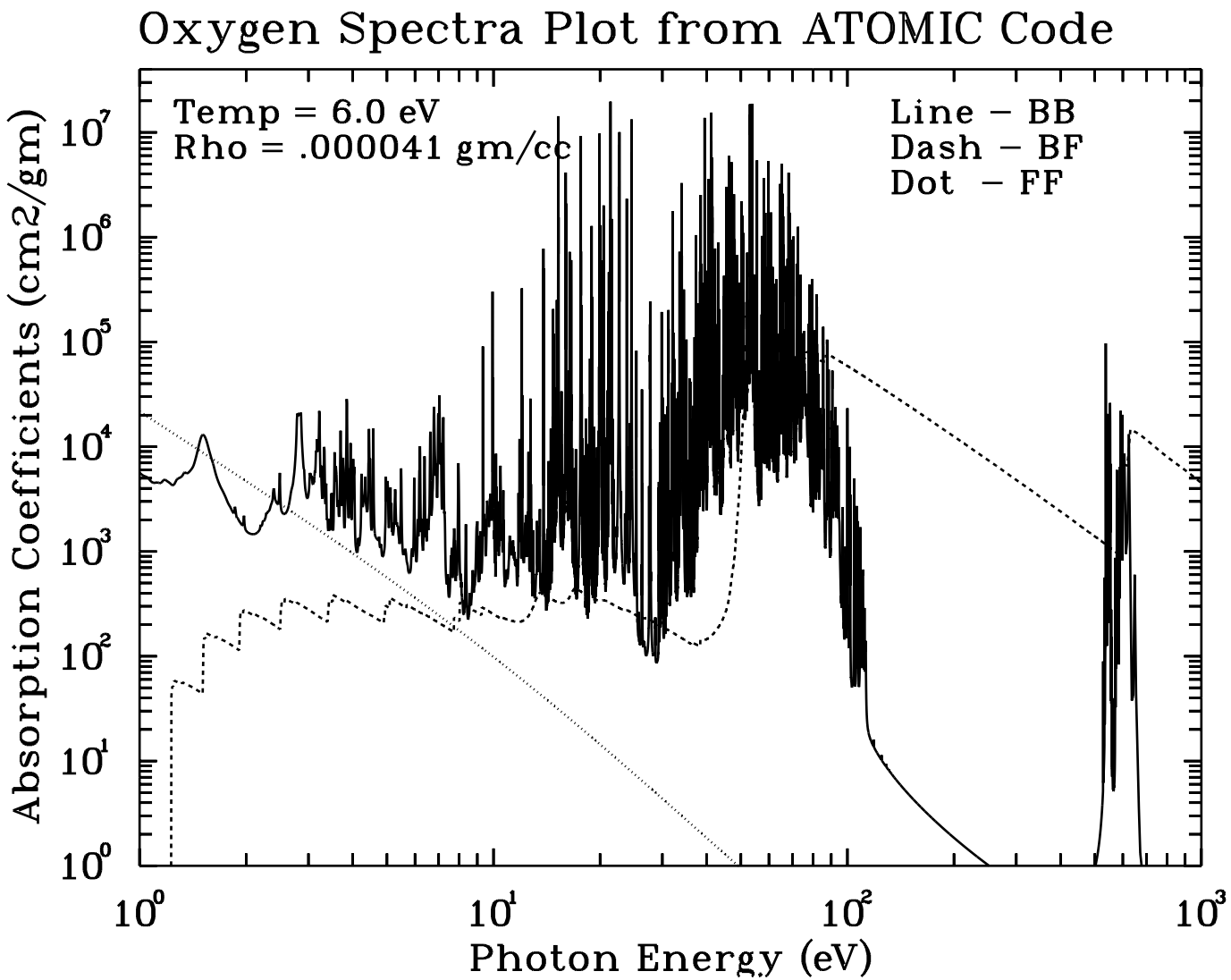
Typical Output Quantities for Comparisons

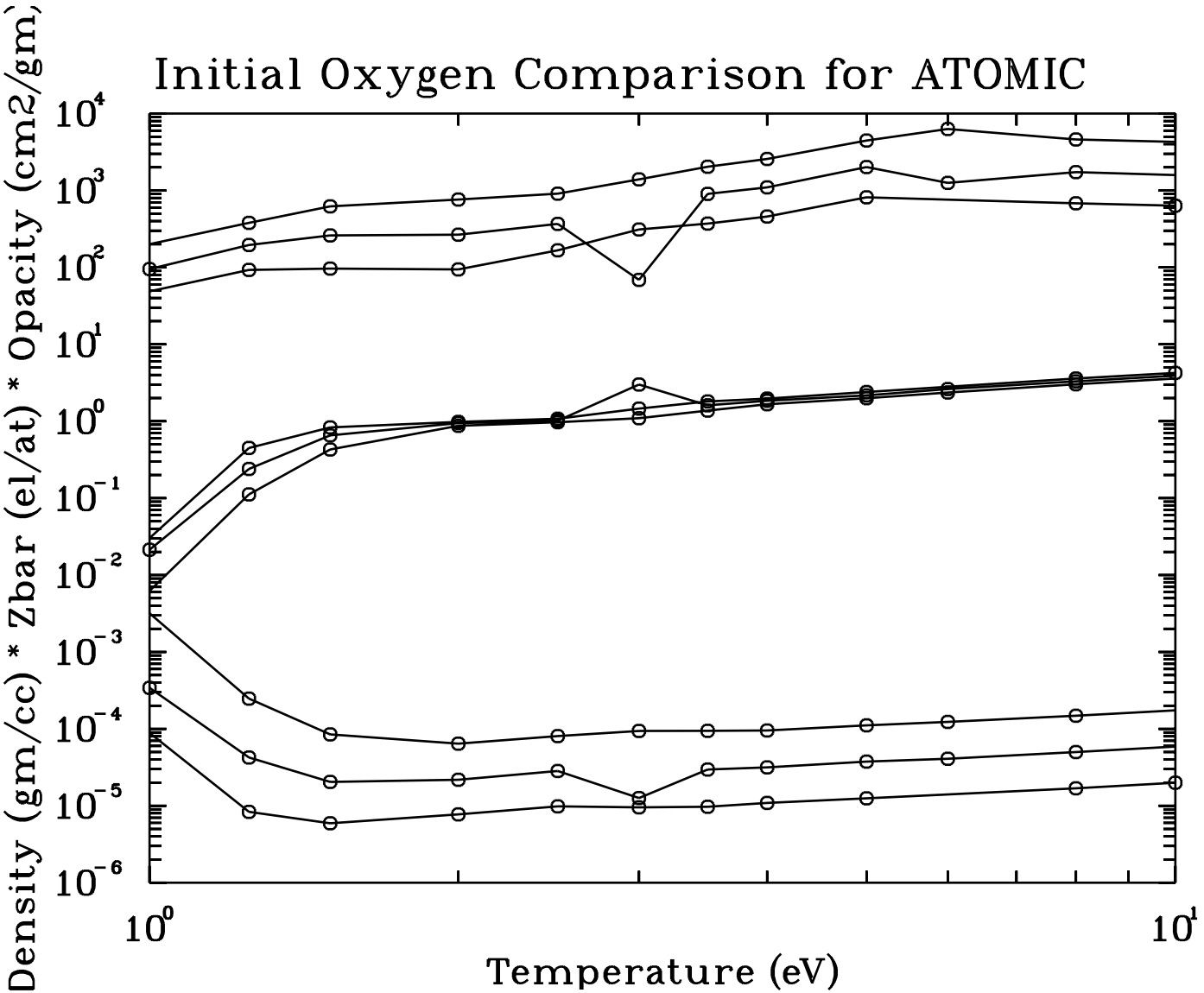
EOS

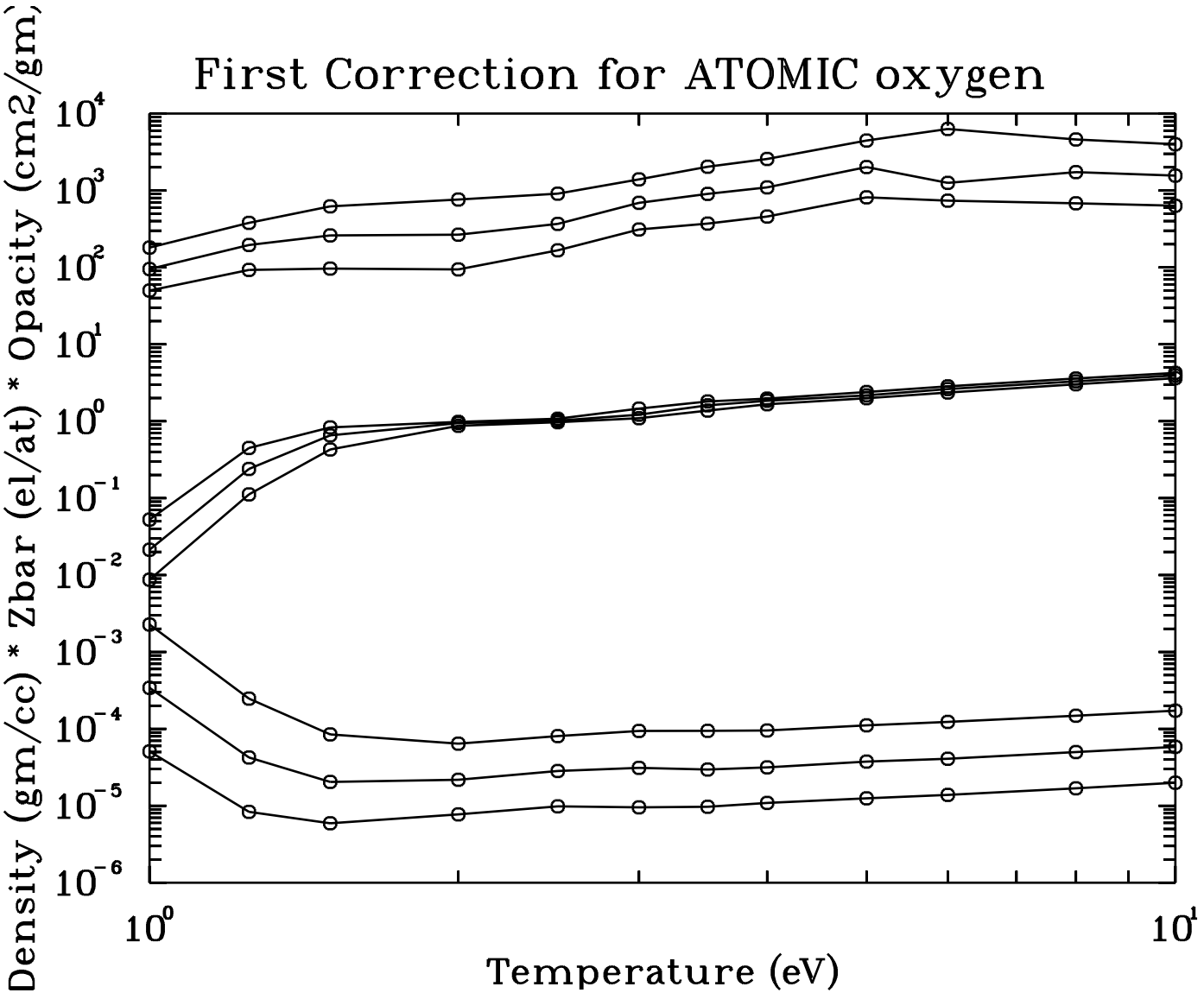
- Zbar
- Electron Density
- Ion Density
- Mass Density
- Pressure (kinetic, plasma, etc. terms)
- Energy (kinetic, plasma, etc. terms)
- Plasma Frequency Cutoff
- Ion & Configuration Abundances

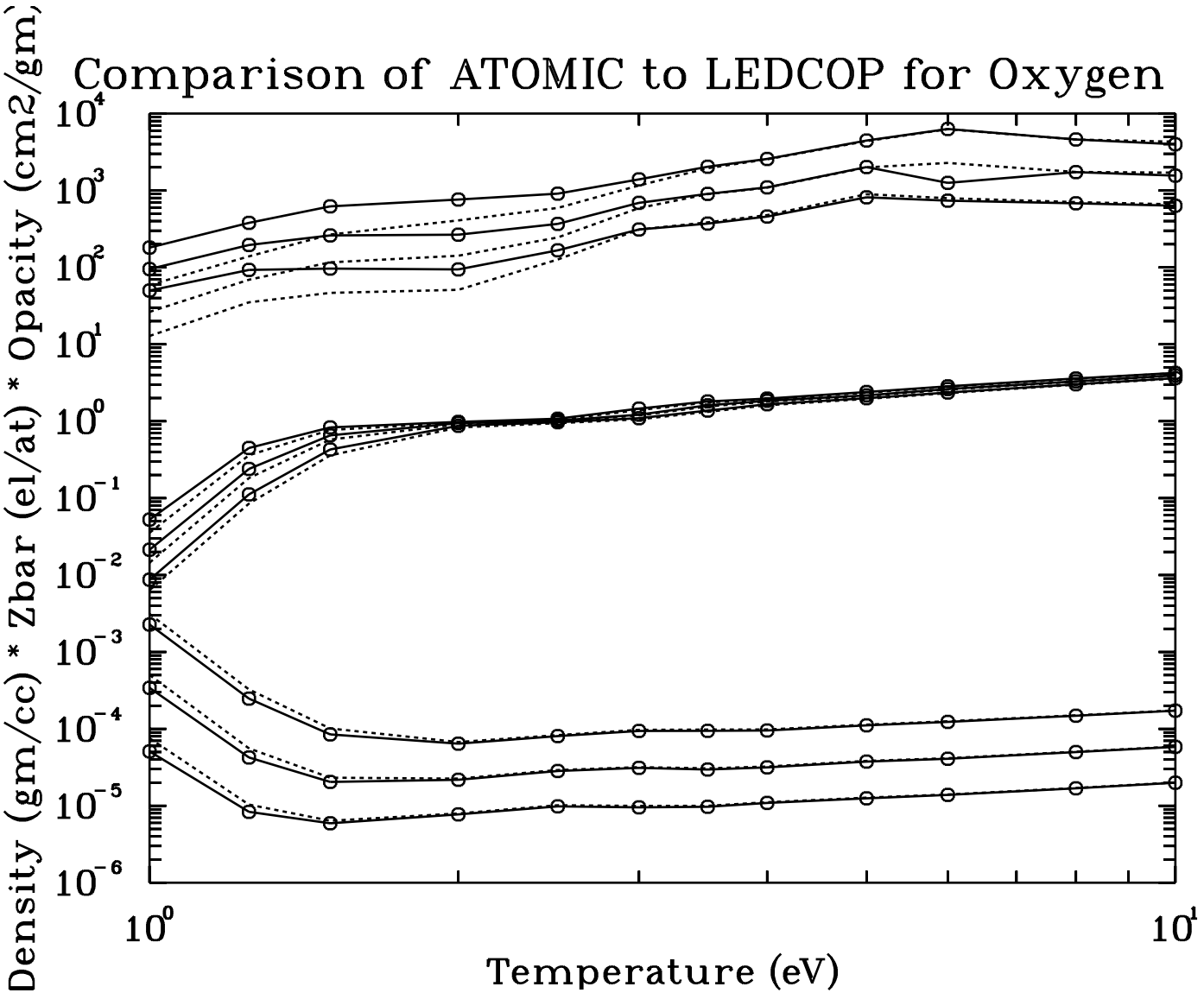
OPACITY

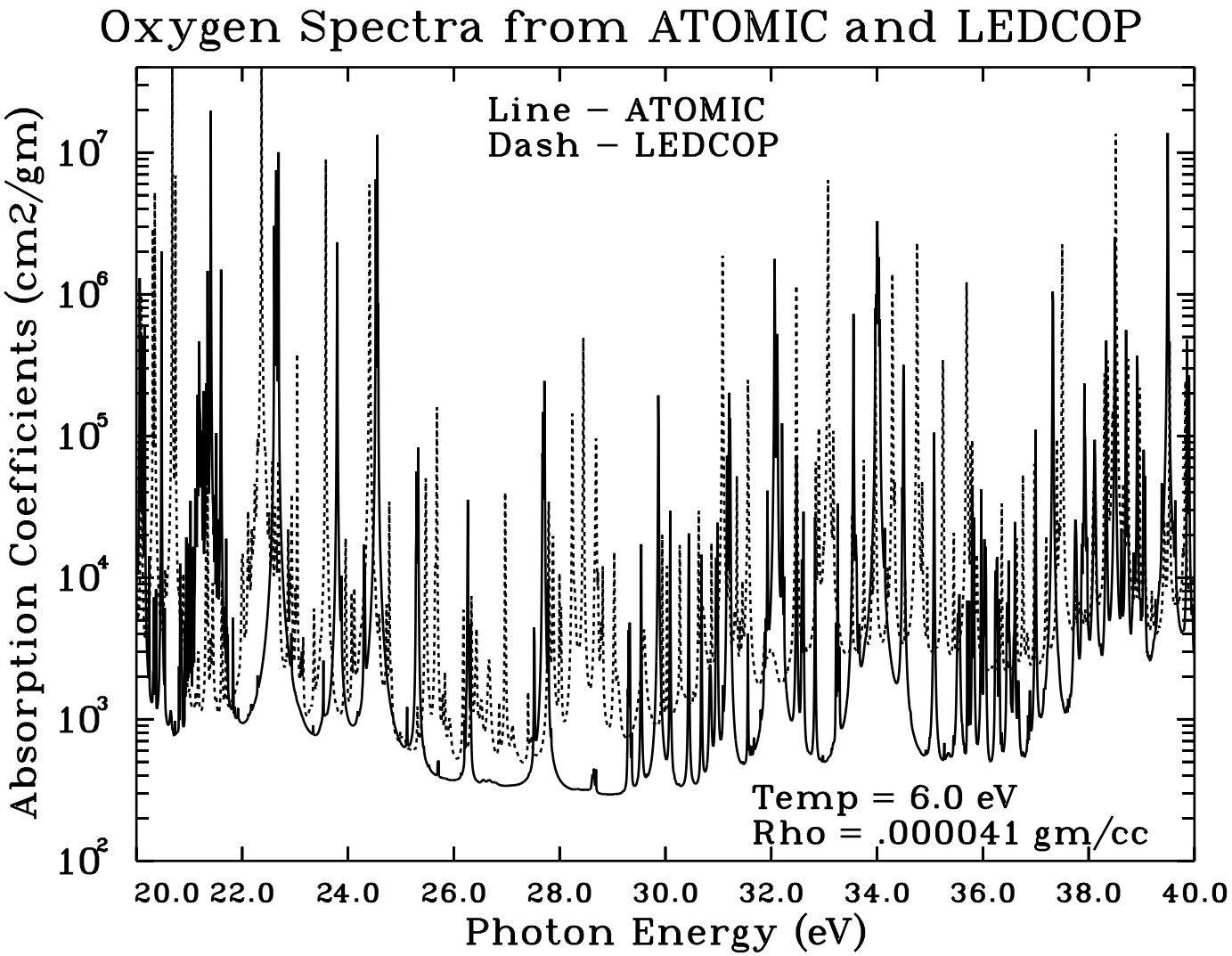
- Continuous & Total Rosseland Opacity
- Continuous & Total Planck Opacity
- Conductive Opacity
- Energy Dependent Opacities
  - ...Total Absorption
  - ...FF Absorption
  - ...BF Absorption
  - ...BB Absorption
  - ...Scattering
- Spectral Idenification

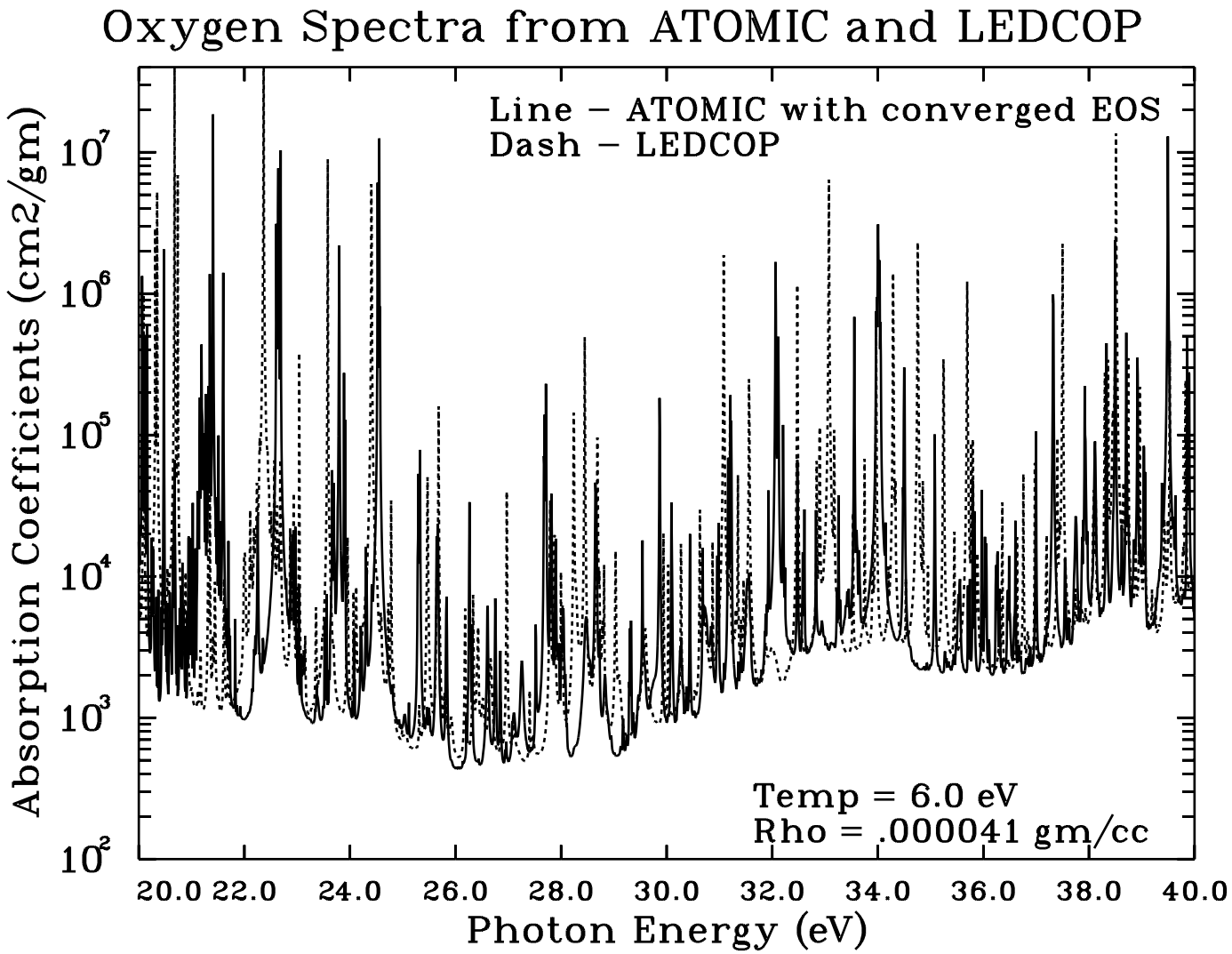

Oxygen Spectra Plot from ATOMIC Code
Temp = 6.0 eV
Rho = .000041 gm/cc
Line – BB
Dash – BF
Dot – FF
Absorption Coefficients (cm2/gm)
Photon Energy (eV)
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7

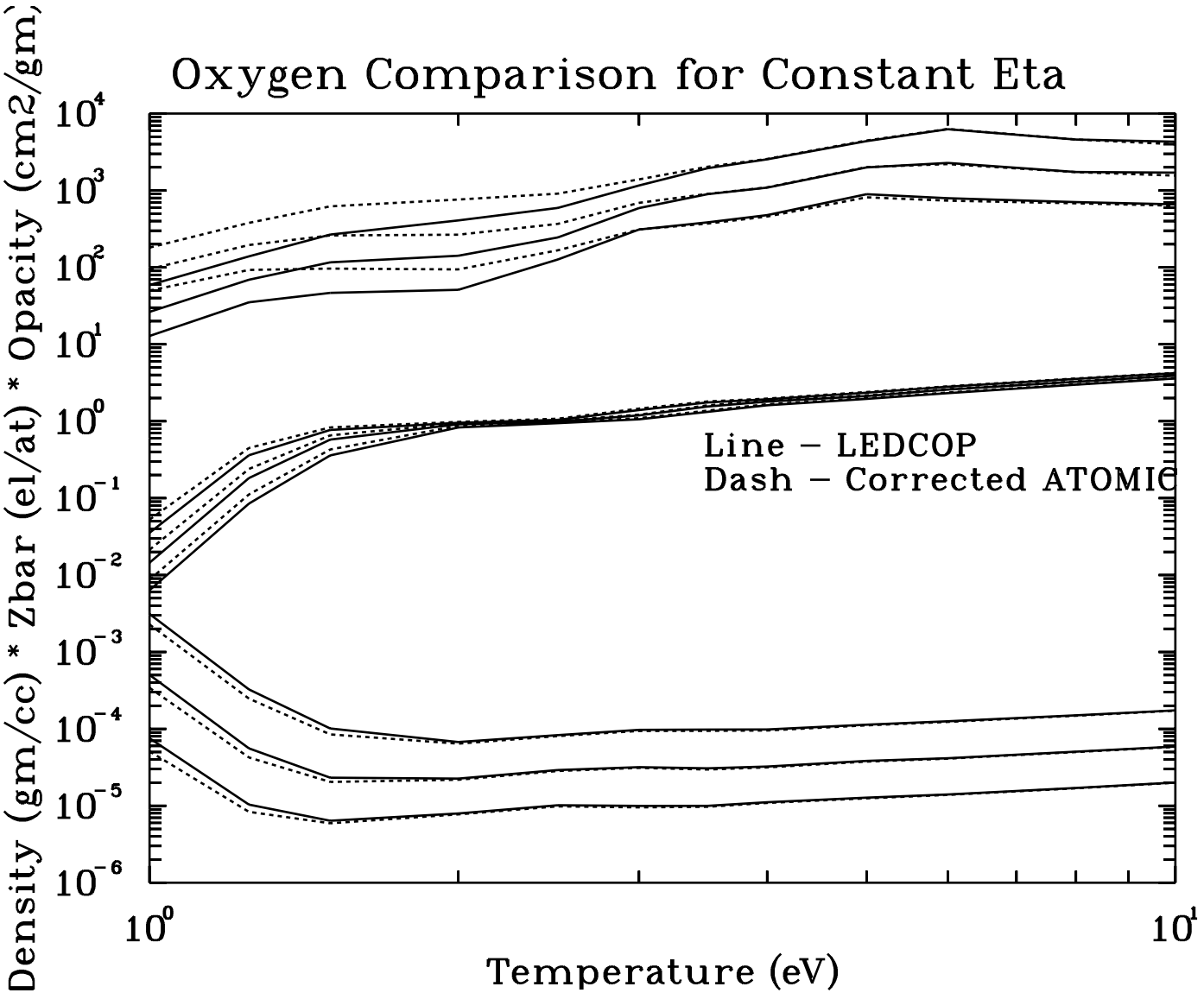

Initial Oxygen Comparison for ATOMIC
Density (gm/cc) * Zbar (el/at) * Opacity (cm2/gm)
Temperature (eV)
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^0
10^1


First Correction for ATOMIC oxygen
Density (gm/cc) * Zbar (el/at) * Opacity (cm2/gm)
Temperature (eV)
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^0
10^1


Comparison of ATOMIC to LEDCOP for Oxygen
Density (gm/cc) * Zbar (el/at) * Opacity (cm2/gm)
Temperature (eV)
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^0
10^1


Oxygen Spectra from ATOMIC and LEDCOP
Line – ATOMIC
Dash – LEDCOP
Temp = 6.0 eV
Rho = .000041 gm/cc
Absorption Coefficients (cm2/gm)
10^7
10^6
10^5
10^4
10^3
10^2
20.0 22.0 24.0 26.0 28.0 30.0 32.0 34.0 36.0 38.0 40.0
Photon Energy (eV)


Oxygen Spectra from ATOMIC and LEDCOP
Line – ATOMIC with converged EOS
Dash – LEDCOP
Temp = 6.0 eV
Rho = .000041 gm/cc
Absorption Coefficients (cm2/gm)
10^7
10^6
10^5
10^4
10^3
10^2
20.0 22.0 24.0 26.0 28.0 30.0 32.0 34.0 36.0 38.0 40.0
Photon Energy (eV)


Oxygen Comparison for Constant Eta
Density (gm/cc) * Zbar (el/at) * Opacity (cm2/gm)
Temperature (eV)
Line – LEDCOP
Dash – Corrected ATOMIC